Design and Performance of Composite Multifunctional Structure-Battery Materials

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ABSTRACT

This paper reports on our development of novel composite multifunctional structure-battery (S-B) materials. We have examined new performance indices and analysis methods in parallel with initial design studies. Several new computational design tools are being used to examine the influence of mesoscale architecture on the structural and energy storage performance of various structure-battery exponent designs.

Keywords: multifunctional, structure-battery, structure-power, composite design

INTRODUCTION

Multifunctional materials are developed to achieve system-level performance enhancements with secondary concern for local subsystem performance. System-level optimization may even result in non-optimal local subsystem design [1]. The multifunctional design paradigm requires a redefinition of existing performance indices to determine the effectiveness of a given multifunctional material system. Presently, the material design space is limited to morphological and compositional arrangement of individual components, each of which provides a unique functionality. The design problem is interdisciplinary with multiple objectives and multiple constraints. The efficacy of the multifunctional approach can be determined by comparing indices of system performance between the multifunctional and baseline (unifunctional structure and battery) designs [1].

The decision of introducing multifunctionality in the design process or even in an existing design is based on the relationship between the targeted system level performance index and various sub-system design parameters. Feasibility of the multifunctional design will also depend on the mutual interfacing capability or physical compatibility of the desired combination of sub-system functions. The example of an electric-motor propelled unmanned air vehicle (UAV) illustrates these points clearly for the case of multifunctional structure-power design [2].

The focus of this paper is on structure-battery (power) multifunctional composite materials that simultaneously provide load-bearing and electrical power storage capabilities. This material system is comprised of a high performance battery system with special packaging and structural additives that provide reasonable mechanical performance. The idea is to replace passive, unifunctional structure with multifunctional structure-power material to increase the operational time or the power output depending upon the targeted application.

In many cases, the mechanical and energy-storage properties of a multifunctional structure-battery material (e.g., specific stiffness, strength, and energy) may not meet the levels that can be achieved by "highly optimized" unifunctional structure and battery materials. Regions of structure or battery that are "underutilized", in a mechanical or energetic sense, are candidate regions for the insertion of power or structure-function materials to achieve structure-power multifunctionality. The highest gains in performance from multifunctionality require implementation of a multifunctional design philosophy right from the start guided by "global" optimization for system performance.

The composite nature of the existing multifunctional structure-battery materials [1,2] limits the applicability of the homogeneous (unifunctional) material performance indices defined by Ashby and coworkers [3,4,5,6], which are suitable for 1-D applications such as beams. General performance parameters that may be important for structure-battery materials such as specific stiffness and energy capacity are well understood for unifunctional structure and battery materials but need to be carefully reconsidered when applied to a multifunctional structure-battery material system.

The arrangement of paper is as follows. Firstly, we discuss the development of multifunctional structure-battery performance indices and briefly outlines our optimization strategy with the help of design selection charts. Following that, we describe a software design tool that calculates a variety of mechanical and energy storage properties for use in ranking structure-battery material designs. Next, we present a design study of circular and square structure-battery struts to examine the effects of shape, material properties, and placement on structure-battery performance. The paper closes with a brief summary of the work.

MULTIFUNCTIONAL STRUCTURE-BATTERY DESIGN APPROACH

A wide variety of structure and battery materials can be "joined" to form multifunctional material systems. The ability to store energy in a chemical state and releasing it on demand as electrical energy is critically sensitive to the component materials and arrangements compared to the dependence of the ability to resist mechanical deformation under loading on these parameters. It makes sense, therefore, to enhance the structure-function of an existing battery material/system rather than trying to add electrical energy storage function to a structure material. Hence, the following multifunctional design rule: ***add functionality to the more complex material/function***.

We assume that the mechanical deformations of a structure-battery does not appreciably affect the energy storage capabilities of the battery material, and that the integrated structural materials are "energetically inert" but add volume and weight to the multifunctional system.

The selection of a battery material for the multifunctional structure-battery system must be guided by the potential improvement in system performance. Desired features and constraints must also guide the selection. For example, in battery-powered UAV's, the common system objective is to maximize the flight-time endurance or range. This constrains the selection to high specific energy battery systems with the potential for moderate structural enhancement. Desired features include: capability for easy incorporation into UAV structure, good reliability over the operating conditions and temperatures, robust handling durability, rechargeability, and safe, non-toxic failure when punctured or electrically shorted.

The potential for moderate structural enhancement and the capability of fabricating structure-battery material to arbitrary shapes are probably the two most common requirements for multifunctional structure-battery implementations. Many battery systems have active elements (anode-separator-cathode) that are configured in thin-sheet laminate form. This is significant in that thin-sheets have the potential for being cut and molded into any desired shape. The active layers can be bonded with the battery cell packaging and additive structural layers for mechanical enhancement and for interfacing to the system structure. In other words, structure-battery materials generally take the form of a laminate composite comprised of various layers of structure and bonding materials, active battery elements, and battery cell packaging. ***Selecting the material components and their mesoscale arrangement or "architecture" is the principal design challenge in the development of an optimally configured multifunctional structure-battery material.***

Mechanical Performance Indices for Structure-Battery Materials

An analysis of mechanical performance of prismatic laminates or layered composite beams can be performed using classical "Mechanics of Materials" equations extended by "modulus-weighted" cross-section properties [7]. We have developed a variety of structural performance indices for composites utilizing this methodology [1,2,10]. To illustrate, we define specific axial stiffness by:

$$p_a := \frac{k_a}{\rho} L \tag{1}$$

where L is the beam length, and k_a is an elastic stiffness and ρ the composite's weight density. The latter two quantities are defined by:

$$k_a := \frac{E_R A^*}{L} \quad \text{where} \quad A^* = \sum_{i=1}^{n} \frac{E_i}{E_R} A_i, \tag{2}$$

$$\rho := \sum_{i=1}^{n} \frac{A_i}{A_T} \rho_i \tag{3}$$

In Eqs. (2)-(3), A^* is the modulus-weighted area, E_R is the reference modulus, n is the number of materials in the cross-section, E_i is the axial modulus, A_i the cross-sectional area and ρ_i the material density of the i^{th} material, and A_T is the sum of the individual material cross-sectional areas. Specific stiffness in tension is then given by:

$$p_a := \frac{k_a}{\rho} L = \frac{E_R \sum_{i=1}^{n} \frac{E_i}{E_R} A_i}{\sum_{i=1}^{n} \rho_i A_i} = \frac{\sum_{i=1}^{n} E_i A_i}{\sum_{i=1}^{n} \rho_i A_i} \tag{4}$$

The performance index in Eq. (4) shows a general dependence on both material properties and architecture; namely, the number of constituents and their shapes, material properties, and cross-section locations. For a single homogeneous material, this simplifies to E / ρ. The dependence of Eq. (4) on both material and architecture variables provides both an opportunity and a challenge. The additional freedoms in the design of the material provide an opportunity for achieving superior performance through architectural arrangement. However, determining the optimal selection of materials and their arrangement is a rather challenging problem.

Energy Storage Performance Indices for Structure-Battery Materials

There are a variety of factors that play a role in a battery cell's energy storage process [8]. Two widely used performance indices include specific energy, e (energy per unit weight), and energy density, E (energy per unit volume). Figure 1 is a plot of ***energy density*** versus ***specific energy*** for a number of technically important primary and secondary battery systems. The data consist of volume and weight normalized energy storage capacity, and these typically depend on the rate of discharge (power draw rate) and operating temperature. This variability in performance is reflected through the use of the "box-point" ranges shown in Figure 1.

The amount of energy that can be stored and delivered by the battery depends on the nature of the active (anode and cathode) materials used in the cell (this determines the voltage) and the amount of active materials present (this determines the Ah capacity). Only a fraction of the theoretical energy storage capacity is realized in practice. The essence of a battery cell is the cathode-electrolyte/separator-anode. Actual battery cells also require cathode and anode current collectors (good conductors), cell packaging, and terminal electrodes. These latter "materials of construction" add non-energy-storing weight and volume to the battery thereby decreasing the apparent performance. The same is true of the structural additive materials in the structure-battery implementation. The exact nature and amount of these structural additive and construction materials depends on the mechanical and electrical operational requirements, battery chemistry, overall geometry, and operating environment.

There are several tests for characterizing the energy storage performance of battery systems including controlled current and power discharge (constant or programmed) with voltage recorded as a function of time. Controlled power discharge tests are used to generate "Ragone plots" that characterize the energy storage capacity versus power discharge rate. A schematic Ragone plot for three battery cells is shown in

Figure 2. Note that the available energy decreases as the rate of discharge increases. Curves A and C correspond to identical cells tested at different temperatures. Curves A and B show the difference between a cell optimized for high-energy storage capacity (curve A) versus a cell optimized for high-power discharge rates (curve B).

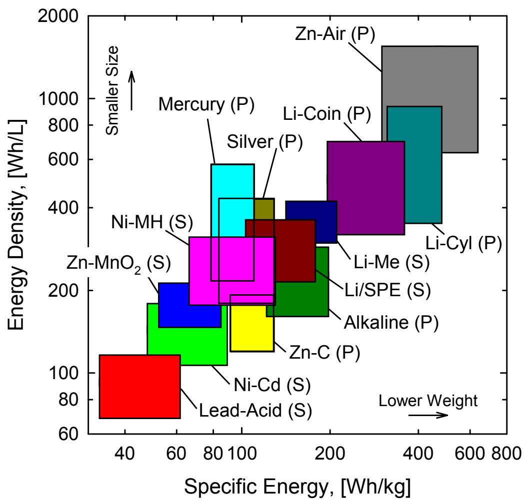


Figure 1: Energy storage capacity of a variety of primary (P) and secondary (S) battery systems normalized with respect to volume and weight. The "box" represents the typical variability in performance. Data from Figures 2 and 3 of Ref. [9].

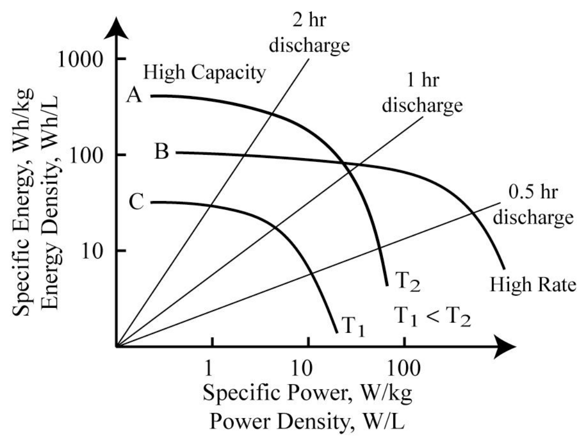


Figure 2: Schematic Ragone plot showing energy storage capacity on a weight or volume basis, for a given power draw rate, again normalized with respect to weight or volume.

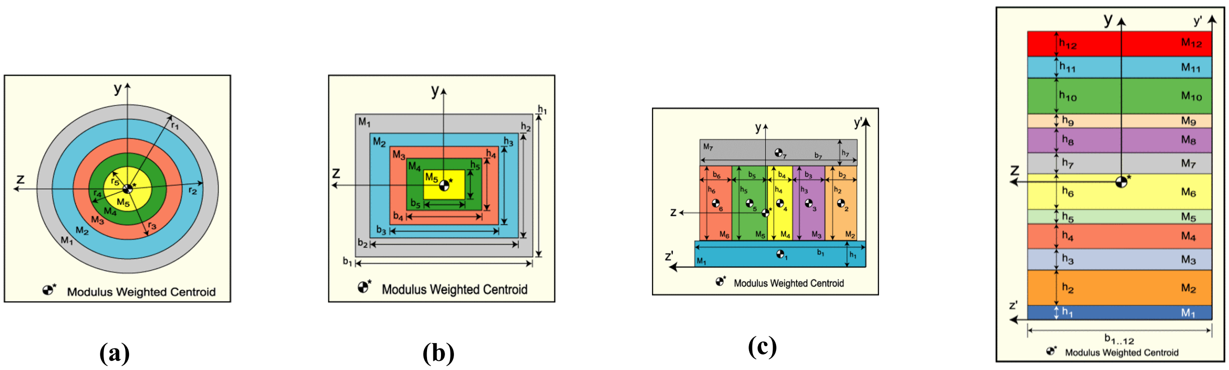
Optimization of Structure-Battery via Material and Architecture

Optimization of structure-battery design depends on both the material (i.e., their number and properties) and architecture (i.e., overall shape and material configuration). In an ideal design analysis, an objective function that is inclusive of all the above-mentioned design parameters will be analyzed for optimum solution under a given set of constraints with the help of analytical and/or computational methods. However, it is usually impossible to find an analytical solution for an all-inclusive objective function. This makes computational methods such as neural networks and genetic algorithms as favored tools for solving optimization problems consisting of a large and multidisciplinary parametric space. The drawback of these methods is the heavy cost of analysis; hence, the goal of initial exploratory studies should be to reduce the size of the parametric space.

We have performed this reduction in the study of structure-battery design by only considering a discrete number of shapes: a) circular-annular, b) rectangular-annular, c) arbitrary-box and d) layered cross-section (Figure 3). Consequently, the remaining independent parameters are the individual materials and their configuration or placement. Ad hoc parametric studies of suitable battery systems with structural additives, and configurations are then carried out by using the structure-battery design tool (SBDT) (described below) to calculate mechanical and electrical energy storage performance. The performance indices for various designs are then plotted on the design selection charts for performance ranking.

COMPUTATIONAL TOOLS FOR STRUCTURE-BATTERY DESIGN

Four computational Structure-Battery Design Tools (SBDT) have been developed at the Naval Research Laboratory for analyzing the mechanical and energy storage performance of composite prismatic beams. The SBDT's are implemented in Excel spreadsheet form [10] and are capable of analyzing: a) circular-annular, b) rectangular-annular, c) arbitrary-box and d) layered cross-section geometries (Figure 3). Inputs include information on component geometries, cross-section locations, and properties. Outputs include: mechanical stiffnesses and strengths for axial, bending, torsion, shear, and buckling loads, volumetric and lineal weight densities, electrical storage capacity, and specific energy and power densities. Nominal electrical performance is calculated assuming constant voltage and currents with complete battery discharge in one hour (i.e., 1C discharge rate†). Each SBDT has two calculation pages. The first, denoted as "Input-Output", performs calculations on a single design. The second page, denoted "Parametric", has each of the entries from the "Input-Output" page arranged horizontally along a single row for performing parametric studies.



(a) (b) (c) (d)

Figure 3: Section configurations that can be analyzed using the Structure-Battery Design Tool (SBDT).

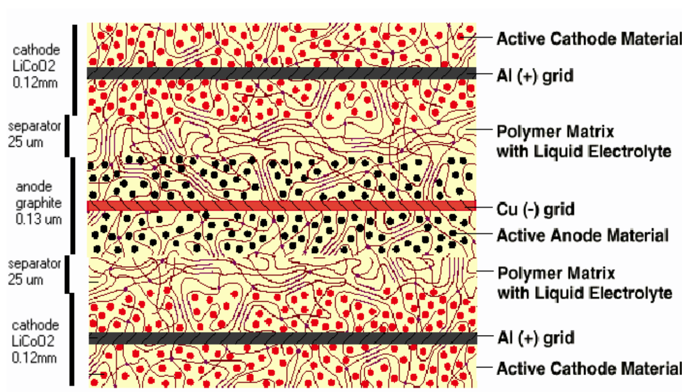


Figure 4: Schematic of the Telcordia plastic-lithium-ion bicell. Total thickness is ~0.5 mm.

SBDT DESIGN STUDY OF STRUCTURE-BATTERY STRUT COMPONENTS

To illustrate an application of the SBDT codes, we report a study on the performance of composite structure-battery struts components with circular and square cross-sections. The SBDT analyses examine the affects of circular versus square shapes, hollow versus solid designs, and non-reinforced versus polypropylene based reinforced configurations on the structure-battery performance. Stiffness and energy storage indices are plotted on the material design selection charts to visualize optimum designs. The battery system that is chosen for the struts is a rechargeable plastic-lithium-ion (PLI) battery system.

† A rate corresponding to "*nC*" is simply a current numerically equal to *n* times the cell's charge capacity, *C*.

PLI battery technology, developed and patented by Telcordia Technologies [11,12] in the early 1990's comes as a bicell in thin (~0.5 mm thick) sheet form (Figure 4). Nominal properties are: 3.8 volt discharge; 7.2 mAh/cm^2 charge storage capacity; and 0.14 g/cm^2 areal weight density. PLI falls under the Li/SPE(S) (lithium/solid-polymer-electrolyte-secondary battery) systems in Figure 1. It is very durable to handling in packaged form, and it is safe (non-toxic, thermal runaway limited) when punctured or electrically shorted. The Li-ion electrolyte used in the bicell is highly reactive with water. Moisture is avoided after imbibing the battery with electrolyte by a laminated polymer/metal chemical barrier layer packaging [2].

Analysis of Two Structure-Battery Strut Components

Ten circular and square cross-section designs comprised of five hollow (A-E) and five polypropylene foam-core (G-K) configurations are considered (Figure 5). Each design contains two layers of PLI bicell to provide approximately equivalent energy-storage capabilities. The cross-sectional area of each design is held constant at 5.067cm^2; the outer diameter for circular cross-section is 2.540cm, and the width/height of the square section is 2.251cm. The results consist of tensile and torsional stiffnesses, and energy content. Normalization with respect to the enclosed volume per unit length and weight per unit length identifies designs that maximize stiffness or energy while minimizing size or weight. The materials properties used in the study are listed in Table 1.

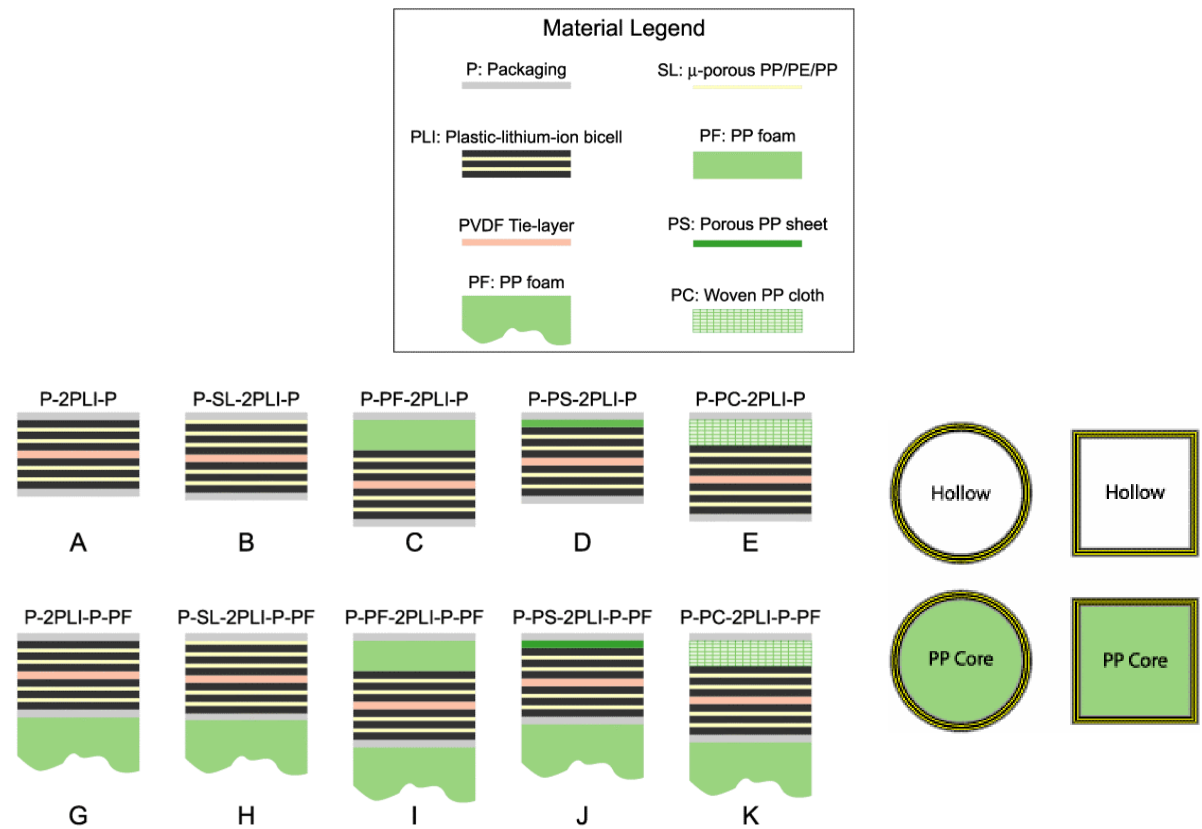


Figure 5: Legend and material section schematics for the circular and square structure-PLI struts analyzed for mechanical and electrical performance using the Structure-Battery Design Tools.

Figure 6 is material design selection chart showing tensile and torsional stiffnesses, normalized with respect to volume (density) and weight (specific), for the circular and square designs. The circular cross-sections perform better (i.e., larger tensile stiffness per unit volume or weight) than the square design, and foam-core designs generally perform better than the hollow counterparts. For the circular cross-sections, designs H, K, and G perform well; design G is best for the square cross-section. Recall that designs H and K use a reinforcing layer of microporous PP or PP cloth with PLI+packaging+PP foam, and design G is simply PLI+packaging+PP foam. There is some overlap between foam-core and hollow designs for torsional performance. Some sort of foam-core would be advised in any design to help prevent localized buckling within the constituent layers.

Table 1: Materials and their structural properties employed in structure-battery composite strut design.

Material	Thickness (cm)	Density (g/cm^3)	Modulus (MPa)	Strength (MPa)
Dai-Nippon EP-40 Laminate Packaging	0.011	1.29	4390	16.8
Fagerdala "Fawolit" Polypropylene Sheet (porous)	0.01	0.048	112	0.9
Fibermat EL-238 Woven Polypropylene Reinforcement Cloth	0.045	0.149	349	27
Telcordia Plastic Lithium-Ion Bicell	0.054	2.5	1020	3.9
Celgard 2300 PP/PE/PP Microporous Sheet	0.003	0.47	1690	10.5
Fagerdala "Fawocel" Polypropylene Foam	variable	0.024	56	0.33

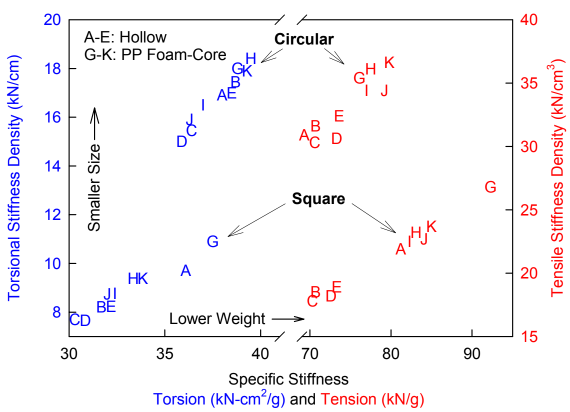


Figure 6: Torsional and tensile stiffness plots for the designs shown in Figure 5.

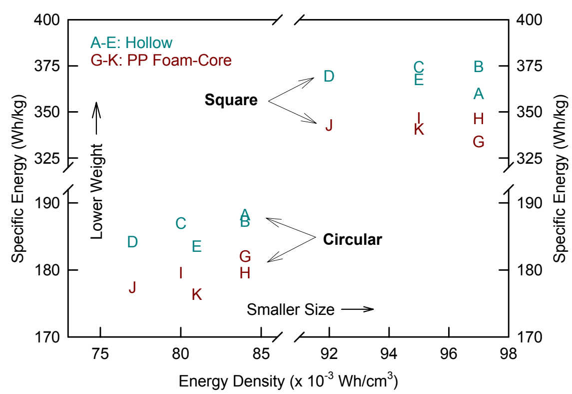


Figure 7: Energy storage capacity plots for the designs shown in Figure 5.

Figure 7 is a material design selection chart showing stored energy normalized with respect to volume (density) and weight (specific) for the ten configurations. The stored energy density values are directly proportional to the amount of PLI bicell material present in the composite. The square cross-sections show higher specific energy than the circular cross-sections; the same ranking follows for hollow versus foam-core designs.

The following points can be summarized:

- Circular struts generally exhibit larger tensile and torsional stiffnesses per unit volume or weight than the square struts.
- The foam-core struts (both circular and square) exhibit better tensile performance than the hollow struts; there is overlap in the torsional performance between the hollow and foam-core struts.
- Square struts contain larger energy per unit weight than the circular struts.
- Hollow struts possess larger energy per unit weight than the foam-core struts.
- PP cloth (PC) and microporous PP (SL) reinforced struts generally exhibit better stiffness values than do struts reinforced by porous PP sheet (PS) or PP foam (PF).

SUMMARY

Concepts associated with the design of multifunctional structure-battery materials have been presented in this paper. The motivation for the development of these types of materials and appropriate design tools is the ***enhancement of system performance***. The use of material performance indices and material design selection charts has been extended to composites. Structure-battery performance indices are established. Several Excel computational design tools have been developed to provide a design ranking capability for multifunctional structure-power materials. The tools are demonstrated in a study of composite circular and square cross-section struts composed of the Telcordia PLI bicell battery material and structural additives.

ACKNOWLEDGEMENTS

The authors gratefully acknowledge the support of Dr. Leo Christodoulou in the DARPA Defense Sciences Office for providing funding under the Synthetic Multifunctional Materials Program. Partial support for this work through NRL 6.1 core research funding is also gratefully acknowledged.

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